

```

1  #-*- coding: utf-8 -*-
2  """
3  Created on Mon Mar 25 14:16:41 2019
4
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6  """
7
8  import numpy as np
9  import matplotlib.pyplot as plt
10 import pdb
11
12
13
14 delta_r = .01
15 l_orbital = [0,1,2,3]
16 #l_orbital = [0]
17 eps_list = []
18
19 #-1/r potential energies
20 #for i in range(1001):
21 #    eps_list.append(i*.001-1)
22
23
24 #r*r/2 potential energies
25 for i in range(1001):
26     eps_list.append(i*.01)
27
28 #u(r-dt), u(r), l, r, eps
29 def stepping(u_2, u_1, l, r, eps):
30     fun = 2*(r*r/2) + l*(l+1)/r**2 - 2*eps
31     #fun = -2/r + l*(l+1)/r**2 - 2*eps
32     u_3 = 2*u_1 - u_2 + delta_r**2*fun*u_1
33     return(u_3)
34
35
36
37 #####
38 #####
39
40
41 good_points = []
42
43 for l in l_orbital:
44     for eps in eps_list:
45         u = [0, .01]
46         r = delta_r*2
47         #
48         #
49         for i in range(5000):
50             u.append(stepping(u[-2], u[-1], l, r, eps))
51             #
52             if u[-1]*u[-2] < 0:
53                 good_points.append([l, eps, r])
54             #
55             r+=delta_r
56             u = [u[-2], u[-1]]
57             #
58
59 #####
60 #####
61 #Plotting
62
63
64 l0 = []
65 l1 = []
66 l2 = []
67 l3 = []

```

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68
69 for i in range(len(good_points)):
70     if good_points[i][0] == 0:
71         l0.append([good_points[i][1], good_points[i][2]])
72     elif good_points[i][0] == 1:
73         l1.append([good_points[i][1], good_points[i][2]])
74     elif good_points[i][0] == 2:
75         l2.append([good_points[i][1], good_points[i][2]])
76     elif good_points[i][0] == 3:
77         l3.append([good_points[i][1], good_points[i][2]])
78
79
80 fig1, axes1 = plt.subplots()
81 axes1.scatter([l0[i][1] for i in range(len(l0))], [l0[i][0] for i in range(len(l0))])
82 axes1.scatter([l1[i][1] for i in range(len(l1))], [l1[i][0] for i in range(len(l1))])
83 axes1.scatter([l2[i][1] for i in range(len(l2))], [l2[i][0] for i in range(len(l2))])
84 axes1.scatter([l3[i][1] for i in range(len(l3))], [l3[i][0] for i in range(len(l3))])
85 axes1.set_ylabel('Energy')
86 axes1.set_xlabel('r')
87 axes1.set_title("Energy Orbitals", va='bottom')
88 axes1.legend(['l=0', 'l=1', 'l=2', 'l=3'], loc='upper right')
89 plt.show()
90
91
92

```